

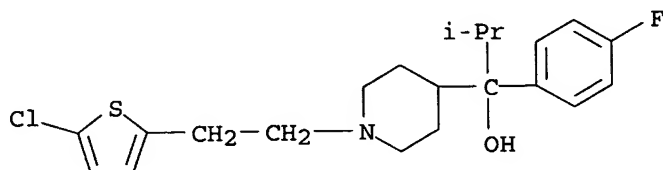
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Match level :
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  11:CLASS 12:CLASS 13:Atom
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    Number of Carbon Atoms : less than 7

Element Count :
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    N,N0-2

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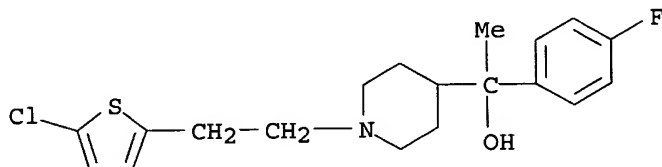
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 FS 3D CONCORD  
 MF C21 H27 Cl F N O S  
 SR CA  
 LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 2 OF 13 REGISTRY COPYRIGHT 2002 ACS  
 RN 325706-34-1 REGISTRY  
 CN 4-Piperidinemethanol, 1-[2-(5-chloro-2-thienyl)ethyl]-.alpha.-(4-fluorophenyl)-.alpha.-methyl- (9CI) (CA INDEX NAME)  
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 LC STN Files: CA, CAPLUS

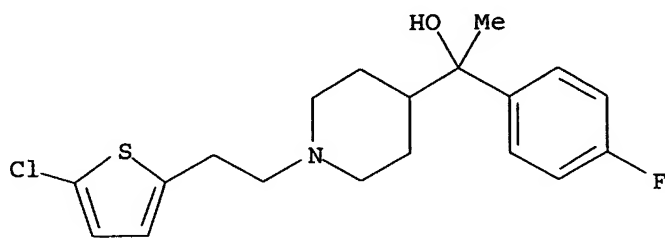


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 3 OF 13 REGISTRY COPYRIGHT 2002 ACS  
 RN 325706-30-7 REGISTRY  
 CN 4-Piperidinemethanol, 1-[2-(5-chloro-2-thienyl)ethyl]-.alpha.-(4-fluorophenyl)-.alpha.-methyl-, hydrochloride, (-)- (9CI) (CA INDEX NAME)  
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 LC STN Files: CA, CAPLUS

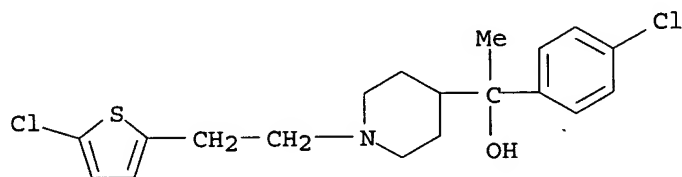
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1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

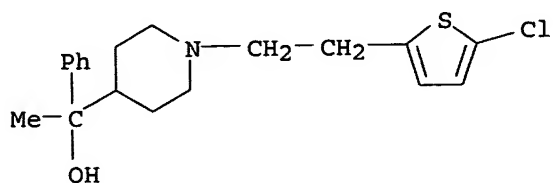
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RN 325706-25-0 REGISTRY  
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MF C19 H23 Cl2 N O S . Cl H  
SR CA  
LC STN Files: CA, CAPLUS



● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)  
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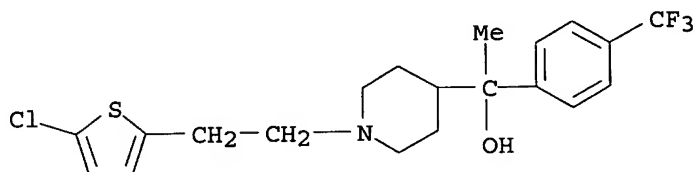
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RN 325706-22-7 REGISTRY  
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SR CA  
LC STN Files: CA, CAPLUS



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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

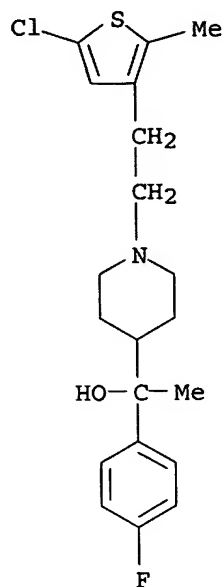
L2 ANSWER 6 OF 13 REGISTRY COPYRIGHT 2002 ACS  
RN 325706-18-1 REGISTRY  
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MF C20 H23 Cl F3 N O S . Cl H  
SR CA  
LC STN Files: CA, CAPLUS



● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

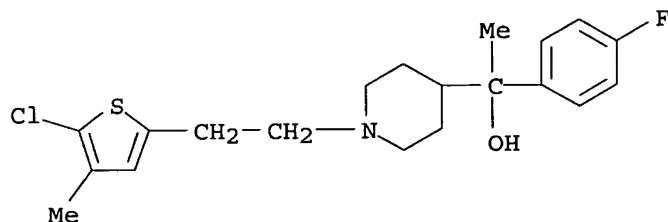
L2 ANSWER 7 OF 13 REGISTRY COPYRIGHT 2002 ACS  
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MF C20 H25 Cl F N O S . Cl H  
SR CA  
LC STN Files: CA, CAPLUS



● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)  
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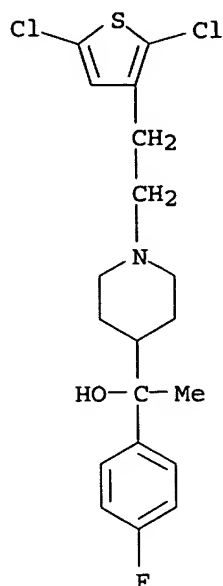
L2 ANSWER 8 OF 13 REGISTRY COPYRIGHT 2002 ACS  
RN 325706-10-3 REGISTRY  
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MF C20 H25 Cl F N O S . Cl H  
SR CA  
LC STN Files: CA, CAPLUS



● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

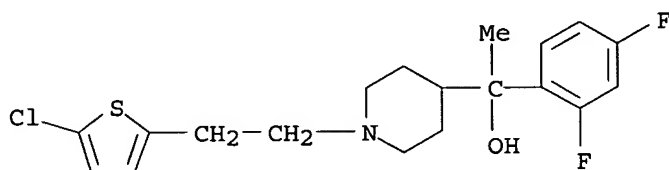
L2 ANSWER 9 OF 13 REGISTRY COPYRIGHT 2002 ACS  
RN 325706-09-0 REGISTRY  
CN 4-Piperidinemethanol, 1-[2-(2,5-dichloro-3-thienyl)ethyl]-.alpha.-(4-fluorophenyl)-.alpha.-methyl-, hydrochloride (9CI) (CA INDEX NAME)  
MF C19 H22 Cl2 F N O S . Cl H  
SR CA  
LC STN Files: CA, CAPLUS



● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)  
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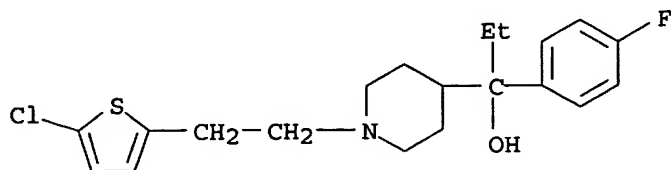
L2 ANSWER 10 OF 13 REGISTRY COPYRIGHT 2002 ACS  
RN 325706-02-3 REGISTRY  
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SR CA  
LC STN Files: CA, CAPLUS



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1 REFERENCES IN FILE CA (1962 TO DATE)  
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L2 ANSWER 11 OF 13 REGISTRY COPYRIGHT 2002 ACS  
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LC STN Files: CA, CAPLUS

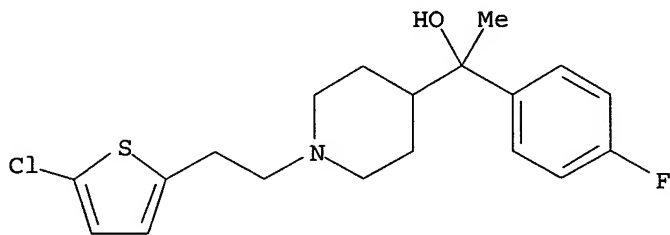


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1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 12 OF 13 REGISTRY COPYRIGHT 2002 ACS  
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CN 4-Piperidinemethanol, 1-[2-(5-chloro-2-thienyl)ethyl]-.alpha.-(4-fluorophenyl)-.alpha.-methyl-, hydrochloride, (+)-(9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C19 H23 Cl F N O S . Cl H  
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LC STN Files: CA, CAPLUS

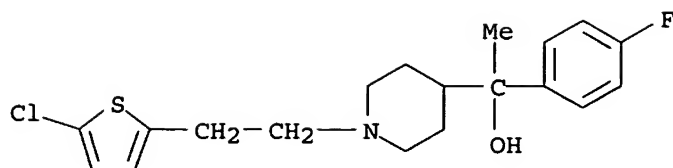
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1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 13 OF 13 REGISTRY COPYRIGHT 2002 ACS  
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MF C19 H23 Cl F N O S . Cl H  
SR CA  
LC STN Files: CA, CAPLUS  
CRN (325706-34-1)



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1 REFERENCES IN FILE CA (1962 TO DATE)  
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L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS

AN 2001:136797 CAPLUS

DN 134:162928

TI Preparation of piperidinyllalkanols as 5-HT2A antagonists.

IN Pruecher, Helmut; Boettcher, Henning; Ackermann, Karl-August; Gottschlich, Rudolf; Greiner, Hartmut; Harting, Juergen; Bartoszyk, Gerd; Seyfried, Christoph; Van Amsterdam, Chrostoph

PA Merck Patent G.M.B.H., Germany

SO Ger. Offen., 18 pp.

CODEN: GWXXBX

DT Patent

LA German

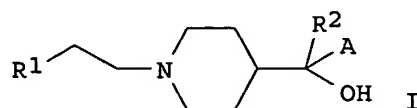
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OS MARPAT 134:162928

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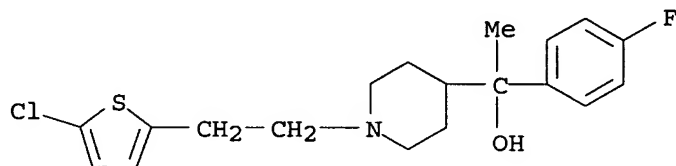
AB Title compds. [I; R1, R2 = (substituted) Ph, heterocyclyl; A = alkyl] and salts or solvates thereof were prepd. for treatment of psychosis, amnesia, eating disorders, etc. Thus, 2-chloro-5-(2-chloroethyl)thiophene, 1-(4-fluorophenyl)-1-piperidin-4-ylethanol HCl, and NaHCO<sub>3</sub> were stirred for 8 h at 80.degree. in MeCN to give 1-[1-[2-(5-chlorothiophen-2-yl)ethyl]piperidin-4-yl]-1-(4-fluorophenyl)ethanol. I showed 5-HT<sub>2A</sub> antagonist effects with IC<sub>50</sub> = 1.5 .times. 10<sup>-10</sup> M to 2.5 .times. 10<sup>-7</sup> M.

IT 325705-90-6P

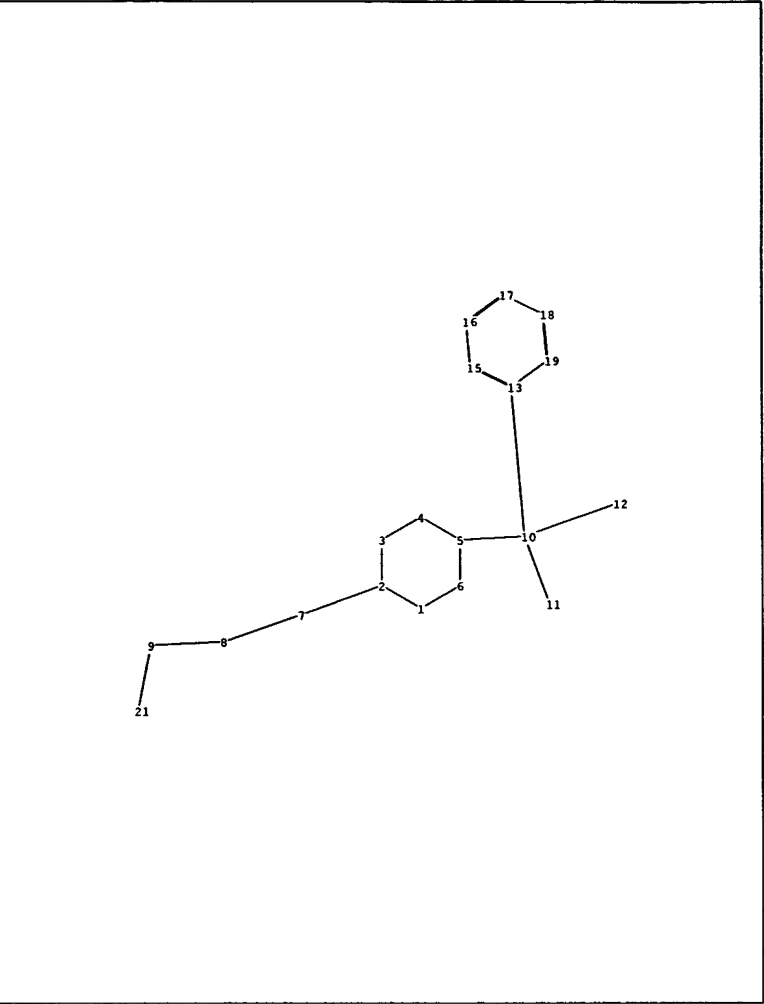
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of piperidine alcs. as 5-HT<sub>2A</sub> antagonists)

RN 325705-90-6 CAPLUS

CN 4-Piperidinemethanol, 1-[2-(5-chloro-2-thienyl)ethyl]-.alpha.-(4-fluorophenyl)-.alpha.-methyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl



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11:CLASS 12:CLASS 13:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 21:CLASS
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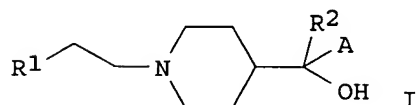
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Saturation              : Saturated
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Node 9: Limited  
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AN 134:162928 CA  
 TI Preparation of piperidinyllalkanols as 5-HT2A antagonists.  
 IN Pruecher, Helmut; Boettcher, Henning; Ackermann, Karl-August; Gottschlich, Rudolf; Greiner, Hartmut; Harting, Juergen; Bartoszyk, Gerd; Seyfried, Christoph; Van Amsterdam, Chrostoph  
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 SO Ger. Offen., 18 pp.  
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 DT Patent  
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 FAN.CNT 1

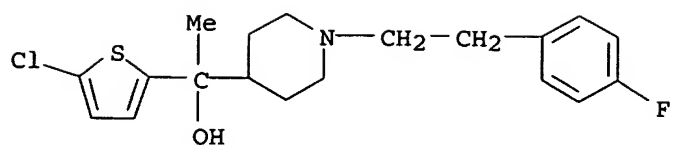
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	WO 2001014332	A1	20010301	WO 2000-EP7664	20000808
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	NO 2002000827	A	20020220	NO 2002-827	20020220
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OS	MARPAT 134:162928				
GI					



AB Title compds. [I; R1, R2 = (substituted) Ph, heterocyclyl; A = alkyl] and salts or solvates thereof were prepd. for treatment of psychosis, amnesia, eating disorders, etc. Thus, 2-chloro-5-(2-chloroethyl)thiophene, 1-(4-fluorophenyl)-1-piperidin-4-ylethanol HCl, and NaHCO3 were stirred for 8 h at 80.degree. in MeCN to give 1-[1-[2-(5-chlorothiophen-2-yl)ethyl]piperidin-4-yl]-1-(4-fluorophenyl)ethanol. I showed 5-HT2A antagonist effects with IC50 = 1.5 .times. 10-10 M to 2.5 .times. 10-7 M.

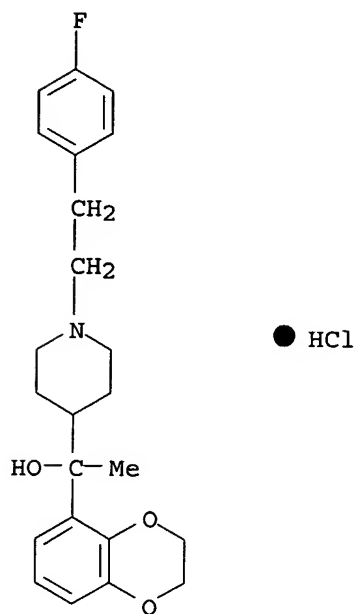
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L8 ANSWER 1 OF 1 CA COPYRIGHT 2002 ACS  
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 (prepn. of piperidine alcs. as 5-HT2A antagonists)  
 RN 325706-24-9 CA  
 CN 4-Piperidinemethanol, .alpha.-(5-chloro-2-thienyl)-1-[2-(4-fluorophenyl)ethyl]-.alpha.-methyl- (9CI) (CA INDEX NAME)



RN 325706-28-3 CA

CN 4-Piperidinemethanol, .alpha.-(2,3-dihydro-1,4-benzodioxin-5-yl)-1-[2-(4-fluorophenyl)ethyl]-.alpha.-methyl-, hydrochloride (9CI) (CA INDEX NAME)



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SAMPLE SCREEN SEARCH COMPLETED - 93 TO ITERATE

100.0% PROCESSED 93 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 1282 TO 2438  
PROJECTED ANSWERS: 0 TO 0

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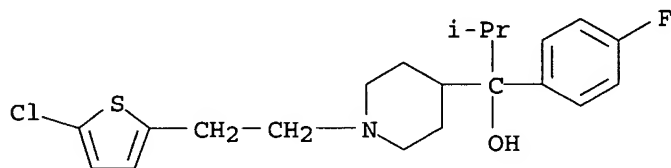
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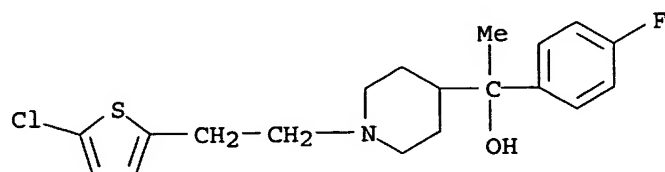
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FS 3D CONCORD  
MF C21 H27 Cl F N O S  
SR CA  
LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 2 OF 9 REGISTRY COPYRIGHT 2002 ACS  
RN 325706-34-1 REGISTRY  
CN 4-Piperidinemethanol, 1-[2-(5-chloro-2-thienyl)ethyl]-.alpha.-(4-fluorophenyl)-.alpha.-methyl- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C19 H23 Cl F N O S  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS

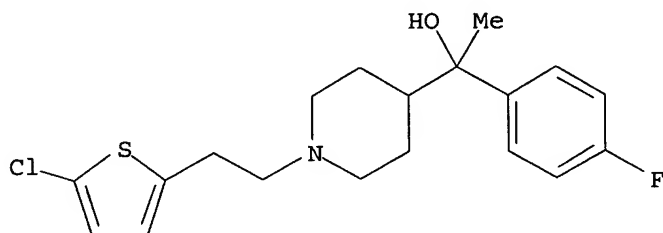


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 3 OF 9 REGISTRY COPYRIGHT 2002 ACS  
RN 325706-30-7 REGISTRY  
CN 4-Piperidinemethanol, 1-[2-(5-chloro-2-thienyl)ethyl]-.alpha.-(4-fluorophenyl)-.alpha.-methyl-, hydrochloride, (-)-(9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C19 H23 Cl F N O S . Cl H  
SR CA  
LC STN Files: CA, CAPLUS

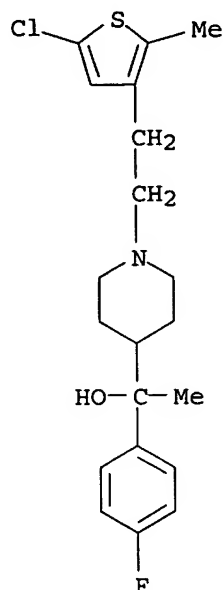
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● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

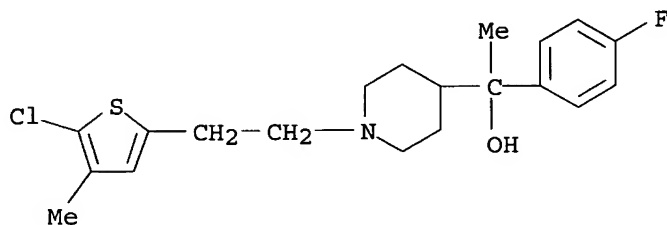
L3 ANSWER 4 OF 9 REGISTRY COPYRIGHT 2002 ACS  
RN 325706-15-8 REGISTRY  
CN 4-Piperidinemethanol, 1-[2-(5-chloro-2-methyl-3-thienyl)ethyl]-.alpha.-(4-fluorophenyl)-.alpha.-methyl-, hydrochloride (9CI) (CA INDEX NAME)  
MF C20 H25 Cl F N O S . Cl H  
SR CA  
LC STN Files: CA, CAPLUS



● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

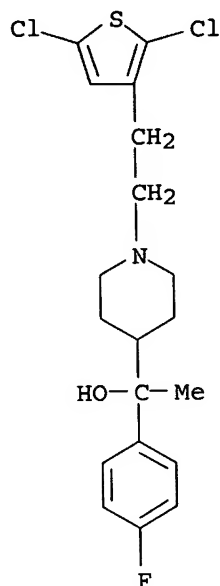
L3 ANSWER 5 OF 9 REGISTRY COPYRIGHT 2002 ACS  
RN 325706-10-3 REGISTRY  
CN 4-Piperidinemethanol, 1-[2-(5-chloro-4-methyl-2-thienyl)ethyl]-.alpha.-(4-fluorophenyl)-.alpha.-methyl-, hydrochloride (9CI) (CA INDEX NAME)  
MF C20 H25 Cl F N O S . Cl H  
SR CA  
LC STN Files: CA, CAPLUS



● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

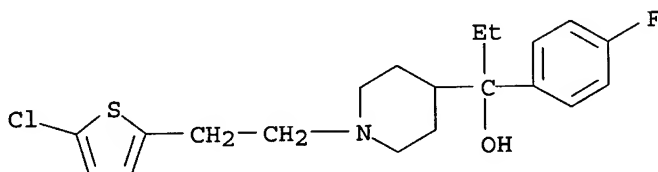
L3 ANSWER 6 OF 9 REGISTRY COPYRIGHT 2002 ACS  
RN 325706-09-0 REGISTRY  
CN 4-Piperidinemethanol, 1-[2-(2,5-dichloro-3-thienyl)ethyl]-.alpha.-(4-fluorophenyl)-.alpha.-methyl-, hydrochloride (9CI) (CA INDEX NAME)  
MF C19 H22 Cl2 F N O S . Cl H  
SR CA  
LC STN Files: CA, CAPLUS



● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 7 OF 9 REGISTRY COPYRIGHT 2002 ACS  
RN 325706-00-1 REGISTRY  
CN 4-Piperidinemethanol, 1-[2-(5-chloro-2-thienyl)ethyl]-.alpha.-ethyl-.alpha.-(4-fluorophenyl)-, hydrochloride (9CI) (CA INDEX NAME)  
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LC STN Files: CA, CAPLUS



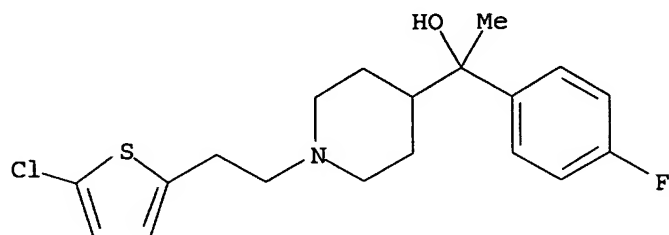
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1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 8 OF 9 REGISTRY COPYRIGHT 2002 ACS  
RN 325705-91-7 REGISTRY  
CN 4-Piperidinemethanol, 1-[2-(5-chloro-2-thienyl)ethyl]-.alpha.-(4-fluorophenyl)-.alpha.-methyl-, hydrochloride, (+)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C19 H23 Cl F N O S . Cl H  
SR CA  
LC STN Files: CA, CAPLUS

Rotation (+).

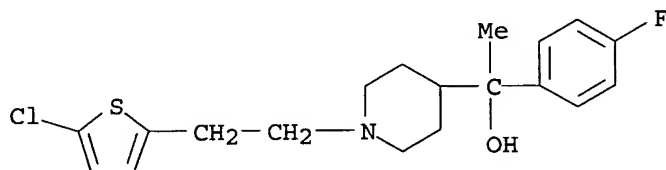




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1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 9 OF 9 REGISTRY COPYRIGHT 2002 ACS  
RN 325705-90-6 REGISTRY  
CN 4-Piperidinemethanol, 1-[2-(5-chloro-2-thienyl)ethyl]-.alpha.-(4-fluorophenyl)-.alpha.-methyl-, hydrochloride (9CI) (CA INDEX NAME)  
MF C19 H23 Cl F N O S . Cl H  
SR CA  
LC STN Files: CA, CAPLUS  
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● HCl

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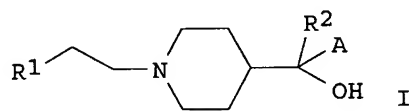
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L4 1 L3

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L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS  
AN 2001:136797 CAPLUS  
DN 134:162928  
TI Preparation of piperidinyalkanols as 5-HT2A antagonists.  
IN Pruecher, Helmut; Boettcher, Henning; Ackermann, Karl-August; Gottschlich, Rudolf; Greiner, Hartmut; Harting, Juergen; Bartoszyk, Gerd; Seyfried, Christoph; Van Amsterdam, Chrostoph  
PA Merck Patent G.M.B.H., Germany  
SO Ger. Offen., 18 pp.  
CODEN: GWXXBX  
DT Patent  
LA German  
FAN.CNT 1  
PATENT NO. KIND DATE APPLICATION NO. DATE

PI DE 19939756 A1 20010222 DE 1999-19939756 19990821  
 WO 2001014332 A1 20010301 WO 2000-EP7664 20000808  
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 IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,  
 MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,  
 SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,  
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 CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
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 EP 1202966 A1 20020508 EP 2000-964004 20000808  
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 OS MARPAT 134:162928  
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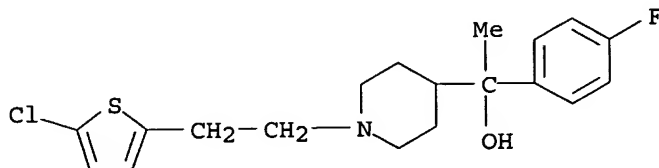
AB Title compds. [I; R1, R2 = (substituted) Ph, heterocyclyl; A = alkyl] and salts or solvates thereof were prep'd. for treatment of psychosis, amnesia, eating disorders, etc. Thus, 2-chloro-5-(2-chloroethyl)thiophene, 1-(4-fluorophenyl)-1-piperidin-4-ylethanol HCl, and NaHCO<sub>3</sub> were stirred for 8 h at 80.degree. in MeCN to give 1-[1-[2-(5-chlorothiophen-2-yl)ethyl]piperidin-4-yl]-1-(4-fluorophenyl)ethanol. I showed 5-HT<sub>2A</sub> antagonist effects with IC<sub>50</sub> = 1.5 .times. 10<sup>-10</sup> M to 2.5 .times. 10<sup>-7</sup> M.

IT 325705-90-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of piperidine alcs. as 5-HT<sub>2A</sub> antagonists)

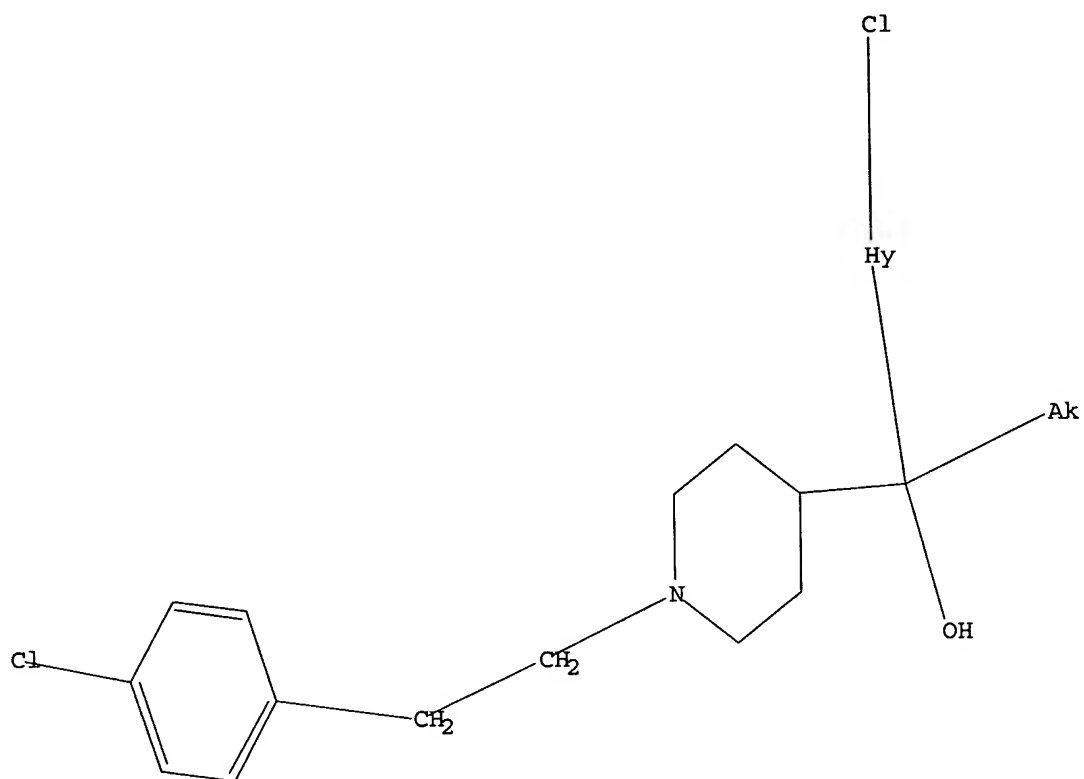
RN 325705-90-6 CAPLUS

CN 4-Piperidinemethanol, 1-[2-(5-chloro-2-thienyl)ethyl]-.alpha.-(4-fluorophenyl)-.alpha.-methyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

=> d  
L5 HAS NO ANSWERS  
L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l5  
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SAMPLE SCREEN SEARCH COMPLETED - 80 TO ITERATE

100.0% PROCESSED 80 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
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PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> s l5 ful  
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FULL SCREEN SEARCH COMPLETED - 1725 TO ITERATE

100.0% PROCESSED 1725 ITERATIONS  
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0 ANSWERS

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Uploading rkc054b.str

L8        STRUCTURE UPLOADED

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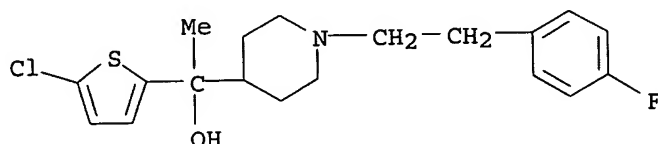
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1 ANSWERS

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L9    ANSWER 1 OF 1    REGISTRY    COPYRIGHT 2002 ACS  
RN    325706-24-9    REGISTRY  
CN    4-Piperidinemethanol, .alpha.-(5-chloro-2-thienyl)-1-[2-(4-fluorophenyl)ethyl]-.alpha.-methyl- (9CI)    (CA INDEX NAME)  
FS    3D CONCORD  
MF    C19 H23 Cl F N O S  
SR    CA  
LC    STN Files:    CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

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L10    ANSWER 1 OF 1    CAPLUS    COPYRIGHT 2002 ACS  
AN    2001:136797    CAPLUS  
DN    134:162928  
TI    Preparation of piperidinylalkanols as 5-HT2A antagonists.  
IN    Pruecher, Helmut; Boettcher, Henning; Ackermann, Karl-August; Gottschlich, Rudolf; Greiner, Hartmut; Harting, Juergen; Bartoszyk, Gerd; Seyfried, Christoph; Van Amsterdam, Chrostoph  
PA    Merck Patent G.M.B.H., Germany  
SO    Ger. Offen., 18 pp.  
      CODEN: GWXXBX

DT    Patent  
LA    German

FAN.CNT 1

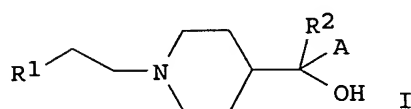
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	WO 2001014332	A1	20010301	WO 2000-EP7664	20000808

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
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CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

BR 2000013467 A 20020430 DE 1999-19939756A 19990821  
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DE 1999-19939756A 19990821  
WO 2000-EP7664 W 20000808  
EP 1202966 A1 20020508 EP 2000-964004 20000808  
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WO 2000-EP7664 W 20000808  
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WO 2000-EP7664 W 20000808

OS MARPAT 134:162928  
GI



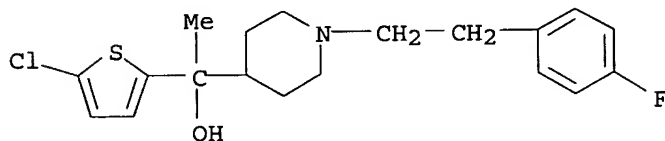
AB Title compds. [I; R1, R2 = (substituted) Ph, heterocyclyl; A = alkyl] and salts or solvates thereof were prepd. for treatment of psychosis, amnesia, eating disorders, etc. Thus, 2-chloro-5-(2-chloroethyl)thiophene, 1-(4-fluorophenyl)-1-piperidin-4-ylethanol HCl, and NaHCO<sub>3</sub> were stirred for 8 h at 80.degree. in MeCN to give 1-[1-[2-(5-chlorothiophen-2-yl)ethyl]piperidin-4-yl]-1-(4-fluorophenyl)ethanol. I showed 5-HT<sub>2A</sub> antagonist effects with IC<sub>50</sub> = 1.5 .times. 10<sup>-10</sup> M to 2.5 .times. 10<sup>-7</sup> M.

IT 325706-24-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of piperidine alcs. as 5-HT<sub>2A</sub> antagonists)

RN 325706-24-9 CAPLUS

CN 4-Piperidinemethanol, .alpha.-(5-chloro-2-thienyl)-1-[2-(4-fluorophenyl)ethyl]-.alpha.-methyl- (9CI) (CA INDEX NAME)



=>

=>

Executing the logoff script...

=> LOG H

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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451.93

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

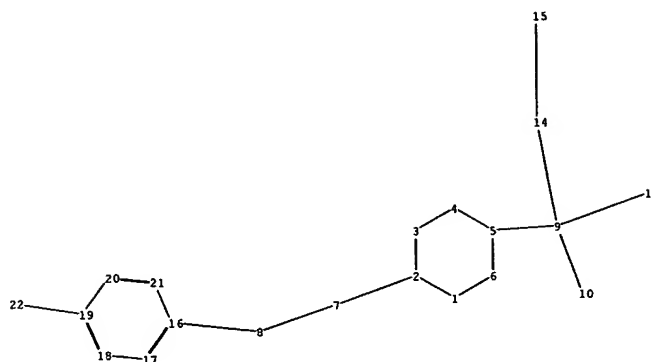
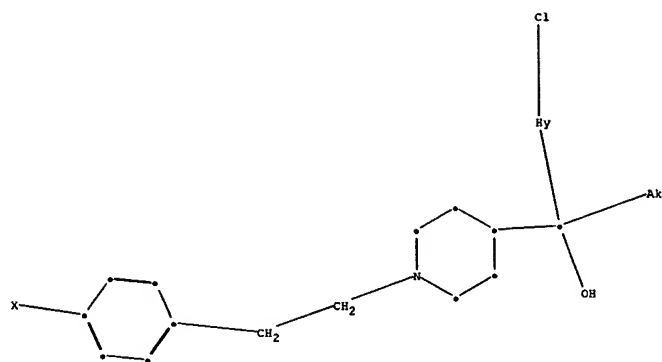
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TOTAL

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CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 60 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 18:40:25 ON 18 DEC 2002



## chain nodes :

7 8 9 10 11 14 15 22

## ring nodes :

1 2 3 4 5 6 16 17 18 19 20 21

## chain bonds :

2-7 5-9 7-8 8-16 9-10 9-11 9-14 14-15 19-22

## ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21

## exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-11 9-14 14-15

## exact bonds :

2-7 5-9 7-8 8-16 19-22

## normalized bonds :

16-17 16-21 17-18 18-19 19-20 20-21

## isolated ring systems :

containing 1 : 16 :

## Hydrogen count :

1:&gt;= minimum 1 3:&gt;= minimum 1 4:&gt;= minimum 1 6:&gt;= minimum 1 17:&gt;= minimum 1

18:&gt;= minimum 1 20:&gt;= minimum 1 21:&gt;= minimum 1

## Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

11:CLASS 14:Atom 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom

22:CLASS

## Generic attributes :

11:

Saturation : Saturated

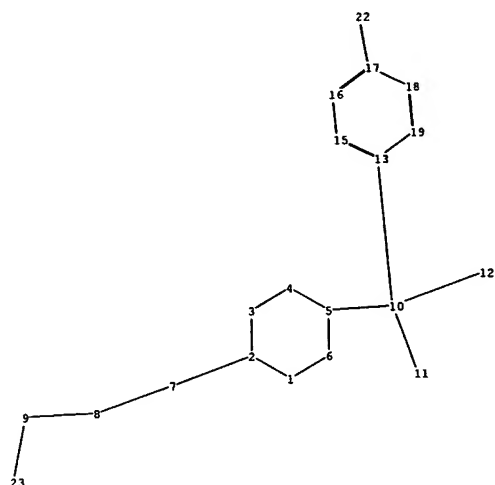
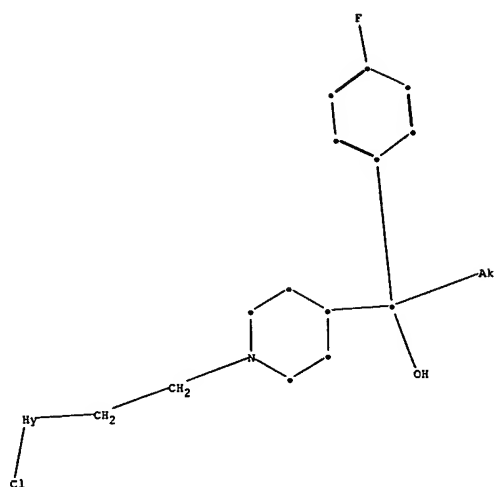
Number of Carbon Atoms : less than 7

14:

Number of Carbon Atoms : less than 7

Number of Hetero Atoms : less than 2

Type of Ring System : Monocyclic



chain nodes :

7 8 9 10 11 12 22 23

ring nodes :

1 2 3 4 5 6 13 15 16 17 18 19

chain bonds :

2-7 5-10 7-8 8-9 9-23 10-11 10-12 10-13 17-22

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-15 13-19 15-16 16-17 17-18 18-19

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 9-23 10-11 10-12

exact bonds :

2-7 5-10 7-8 10-13 17-22

normalized bonds :

13-15 13-19 15-16 16-17 17-18 18-19

isolated ring systems :

containing 1 :

Hydrogen count :

1:>= minimum 1 3:>= minimum 1 4:>= minimum 1 6:>= minimum 1 15:>= minimum 1  
16:>= minimum 1 18:>= minimum 1 19:>= minimum 1

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS  
11:CLASS 12:CLASS 13:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 22:CLASS  
23:CLASS

Generic attributes :

9:

Number of Carbon Atoms : less than 7

Number of Hetero Atoms : less than 2

Type of Ring System : Monocyclic

12:

Saturation : Saturated

Number of Carbon Atoms : less than 7